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A MATHEMATICAL TREATMENT OF THE PROBLEM OF DETERMINING THE EIGENVALUES ASSOCIATED WITH A PARTITION FUNCTION OF AN ATOM IN THE INTERIOR OF A PLASMA

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values for nine different cases.

I. INTRODUCTION

$$
P_i = \begin{vmatrix}
-u_i & e_i & e_2 & \cdots & e_{i-3} & e_{i-2} & e_{i-1} \\
-d_i & -u_{i-1} & e_1 & \cdots & e_{i-4} & e_{i-3} & e_{i-2} \\
O & -d_{i-1} & -u_{i-2} & \cdots & e_{i-5} & e_{i-4} & e_{i-3} \\
\cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\
O & O & O & \cdots & -u_3 & e_1 & e_2 \\
O & O & O & \cdots & -d_3 & -u_2 & e_1 \\
O & O & O & \cdots & O & -d_2 & -u_1
\end{vmatrix} = O, \qquad (6)
$$

where we have set $e_j = \frac{1}{j!}$. The determinant P_i in equation 6 is a polynomial in u of degree i and each root of $b_{i+1} = O$ is a root of $P_i = O$, and conversely. Hence, the two polynomials differ only by a constant multiple. Comparing the leading coefficients, we readily deduce the relation

$$P_i = d_2 d_3 \ \ldots \ d_{i+1} \, b_{i+1}. \tag{7}$$

By a careful analysis of the determinant P_i, it is found that the coefficients of u^i, u^{i-1}, u^{i-2}, and u^{i-3} are respectively

$$(-1)^i \frac{(k+i)!}{\cdots}, \ (-1)^{i-1} \frac{(k+1)!}{\cdots} \sum^{i} \frac{1}{\cdots}$$

which simplifies to

$$\frac{i(i-1)}{2d(k+i)} + \sum_{j>m} \frac{1}{(k+m)(k+j)};$$

the sum of the squares of the roots is

$$-\frac{i(i-1)}{d(k+i)} + \sum_{1}^{i} \frac{1}{(k+j)^2}$$

since $\sum x_j^2 = (\sum x_j)^2 - 2\sum_{j>m} x_m x_j$. These considerations provide precise information concerning the roots. The roots deviate about the values $\frac{1}{k+j}$ and the deviations have a net sum of zero so that some are positive and some are negative (the positive deviations might be accounted for mostly because of pairs of conjugate imaginary roots). The average deviation of the squares of the roots from the values $\frac{1}{(k+j)^2}$ is $-\frac{i-1}{d(k+i)}$, which definitely suggests the presence of imaginary roots in many cases for $i > 1$. When i is increased by 1, a new root is introduced and the net effect on the sum of the roots is as though the roots of P_{i+1} are $\frac{1}{k+i+1}$ and the roots of P_i. However, each real root of P_i is greater than $\frac{1}{k+i}$ as is verified by an analysis of the determinant P_i, which has a positive value when $u \leq \frac{1}{k+i}$. This may be shown by substituting such a value in P_i for u and successively eliminating the $-d_j$, leaving only positive values down the main diagonal and zeroes everywhere below it; or, in case $u = \frac{1}{k+1}$, one can eliminate all the $-d_j$ except $-d_i$ and, as before, P_i has a positive value. Since the eigenvalues are given by u^2 and $\sum^{i} u^2 = -\frac{i(i-1)}{d(k+i)} + \sum^{i} \frac{1}{(k+j)^2}$, we have this condition on the potential eigenvalues. The sum of the products of the roots taken three at a time is

$$\sum_{p>j>m} \frac{1}{(k+m)(k+j)(k+p)} + \frac{1}{8d^2} \sum_{1}^{i-2} \frac{j(j+1)(j+2k+1)(j+2k+2)}{(j+k)(j+k+1)(j+k+2)},$$

the second summation having the value $\frac{(i-2)(i+1)}{2}$ when $k=0$, so that the net deviation in this case is $\frac{(i-2)(i+1)}{16d^2}$. Considering all of these facts, there is an indication that for d large, the deviations are small and vice versa, that there are a few large positive deviations in the most recently introduced roots and in the case of conjugate imaginary roots, and that the less recently introduced roots (which are the largest) tend to stabilize slightly below a value $\frac{1}{k+j}$ at the square root of a potential eigenvalue. One might take $u^2 = \frac{1}{(k+j)^2} - \frac{1}{d}$ as an approximation to an eigenvalue since the average deviation of the squares of the roots from the values $\frac{1}{(k+j)^2}$ is $-\frac{i-1}{d(k+i)}$, which approaches $-\frac{1}{d}$ as i becomes infinite. This suggests the inequality $d \geq (k+j)^2$ as a first approximate limit to the number of eigenvalues where d is finite. This will be reconsidered later.

The coefficient $2dxe^{-x}$ of one term in y or equation 2 is approaching zero at a weakly varying rate for extremely large values of x, when compared to the other coefficients. It might be expected that a reasonable approximation would be obtained by treating e^{-x} as a constant, leading to the equation

$$d_{i+1} \; a_{i+1} = [\,(k+i)\; u - e^{-c}\,]\; a_i \tag{8}$$

and the eigenvalues

$$u = \frac{e^{-c_n}}{k+n} \quad ,$$

where the notation c_n indicates that the constant varies with n, which takes into account the fact that 8 is only an approximation to equation 3. Through the first two terms, when e^{-c_n} is expended into a Taylor series, this agrees with the discussion for k=O of Ecker and Weizel provided we take c_n equal to $\frac{1}{d}\;(k+n)^2$. Thus we have as a second estimate to the eigenvalues

$$u = \frac{1}{k+n}\; e^{-\frac{(k+n)^2}{d}} \quad . \tag{9}$$

To check these approximations further, the determinant equation 6 was solved numerically for i = 1, 2, ..., 10. In addition, the values so obtained were further refined by evaluations of the determinants P_{20}, P_{40}, and P_{41}. Finally a routine was devised based on the recursion formula 4 and the calculations made including the cases i = 1, 2, ..., 75. The latter routine was especially efficient, giving information in 75 cases instead of one case and in about one-fifth of the time taken for the one case.

III. CONCLUDING REMARKS

On the basis of the above and other considerations, the following is presented as the best estimate of the values of the eigenvalues

$$u = \frac{1}{k+n} - \frac{k+n}{d} + \frac{(k+n)^3 - 2k(n+1)}{4d^2} \quad . \tag{10}$$

The values u of equation 10 are thought to be a little more than the true values, leading to the implication that the number of eigenvalues are limited by the following inequality

$$2d \geq (k+n)^2 + \left| 2k(n+1)(k+n) \right|^{\frac{1}{2}}, \tag{11}$$

where n is to take positive integral values and satisfy the inequality. The number of eigenvalues is not greater than the maximum such n (this assumes the correctness of the previous remark).

The numerical results obtained as explained above are summarized in the following tabular data. The values taken for d have been used on the basis of numerical convenience in machine computation. The values themselves are not as important as the general magnitude of this parameter, which may take on any non-negative real value. The parameter k, on the other hand, must be a non-negative integer. The tabular data could be expanded on the basis of the techniques already developed. In fact, the predictor equation 10 may be sufficiently accurate for most cases, the truncation error apparently being of the order of d^{-2} (this remark is based on theoretical reasons as well as on the tabular data below).

d = 1000

k = 0	k = 1	k = 2
.99900025		
.49800199	.49800099	
.33034004	.3303384	.33033554
.24601583	.24601383	.24600983
.19503074	.19502823	.19502323
.16071941	.16071640	.16071040
.13594022	.13593672	.13592972
.11712289	.11711888	.11711085
.10228432	.10227976	.10227081
.090234950	.090229537	.090219821
.080219801	.080214067	.080201641
.071725530	.071697400	.071703049
.064500631	.064424424	.064505604

d = 100

k = 0	k = 1	k = 2
.99002475		
.48019431	.48009421	
.30396993	.30381937	.30351756
.21145270	.21125064	.21084493
.15271597	.15246021	.15194527
.12454326	.12285380	.12136559

d = 10

k = 0	k = 1	k = 2
.90228380		
.40339323	.39722151	.37764286

In general, as i increases in P_i, the roots for k and n large make their initial appearance. The tabular data indicates a definite trend in agreement with inequality 11 and equation 10 agrees with the data in a remarkable way, as one may verify by evaluation of u in equation 10. The estimate due to Ecker and Weizel is equivalent to $\frac{1}{n} - \frac{n}{d} + \frac{n^3}{6d^2} - \ldots$, if we take x_0 to be $\frac{n^2}{d}$, which gives the most favorable choice in general. It may be seen from the tabular data that by our choice of x_o, the results are good but do not give an estimate as good as equation 10.

For each such eigenvalue, the eigenfunction F_n is given by the equation

$$F_n = e^{-udx} \sum_{j=1}^{\infty} (-1)^{j+1} b_j x^{k+j} , \qquad (12)$$

where b_1 is an arbitrary constant not zero, $b_{j+1} = P_j \, (d_2 d_3 \ldots d_{j+1})^{-1}$, $d_{j+1} = \frac{1}{2d}$ $j(j+2k+1)$, P_j is the determinant in equation 6, u is determined by equation 10 (approximately), and n satisfies the restriction 11.

REFERENCE

Ecker, G. and Weizel, W., "The Partition Function and Effective Ionization Potential of an Atom in the Interior of a Plasma," Annalen der Physik, 6 Folge, Band 17, 1956, pp. 126-140.